Numer Algor (2008) 49:235–249
DOI 10.1007/s11075-008-9166-y

ORIGINAL PAPER

Numerical evaluation of a fixed-amplitude variable-phase integral

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Received: 31 July 2007 / Accepted: 10 January 2008 /
Published online: 20 March 2008

Abstract We treat the evaluation of a fixed-amplitude variable-phase integral of the form $\int_a^b \exp[ikG(x)]dx$, where $G'(x) \geq 0$ and has moderate differentiability in the integration interval. In particular, we treat in detail the case in which $G'(a) = G'(b) = 0$, but $G''(a)G''(b) < 0$. For this, we re-derive a standard asymptotic expansion in inverse half-integer inverse powers of k. This derivation is direct, making no explicit appeal to the theories of stationary phase or steepest descent. It provides straightforward expressions for the coefficients in the expansion in terms of derivatives of G at the end-points. Thus it can be used to evaluate the integrals numerically in cases where k is large. We indicate the generalizations to the theory required to cover cases where the oscillator function G has higher order zeros at either or both end-points, but this is not treated in detail. In the simpler case in which $G'(a)G'(b) > 0$, the same approach would recover a special case of a recent result due to Iserles and Nørsett.

Keywords Fixed-amplitude variable-phase integral · Stationary phase asymptotic expansions · Highly oscillatory integrands · Series inversion · Steepest descent integration

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1 Introduction

This paper is about the numerical evaluation of integrals of the form

$$I_0 = \int_a^b F(x) \exp[ikG(x)]dx, \tag{1.1}$$

when k is large. We have in mind cases where F and G are straightforward smooth functions, and function values of both are readily available. In Section 2 we provide an environment in which integrals of this nature occur naturally.

Asymptotic expansions (in inverse powers of k) have recently been published for the case in which $G(x)$ is monotonic and has no stationary values in $[a, b]$. The principal result of this paper is an asymptotic expansion,(in half-integer inverse powers of k) valid in the case in which $F(x)$ is constant, $G(x)$ is symmetric about a and about b, $G'(x) > 0$ in (a, b), $G'(a) = G'(b) = 0$, but $G''(a)G''(b) < 0$. The coefficients are readily calculable functions of G and its derivatives at the end-points, and so this expansion can be used to evaluate the integral when k is large. This expansion in given in Theorem 6.1.

For small k such an integral is readily evaluated by using a standard quadrature formula. But for large k this approach may become prohibitively expensive. The difficulty has little to do with the nature of G and F. To see this, we look at a simple, well-known example. Setting $G(x) = 2\pi x$, we find the integral representation of a Fourier coefficient,

$$\hat{\Phi}(k) = \int_0^1 \Phi(x) \exp[2\pi ikx]dx. \tag{1.2}$$

This integrand function is oscillatory, changing sign roughly $2k$ times in the integration interval. Its evaluation using the trapezoidal rule requires at least $2k$ function values, which for large k can be prohibitive. In this simple case the oscillations have constant phase $1/k$; and when $\Phi(x)$ is regular, this can be exploited to provide the classical Fourier coefficient asymptotic expansion (FCAE) in k. (See Theorem 5.2) This in turn can be exploited to provide a less expensive approach to the calculation. But, when $G(x)$ is not linear, the phase of the oscillation varies with x, making direct numerical quadrature even more hazardous, and invalidating the asymptotic expansion of that form. When $F(x)$ is constant, integrals of this type are sometimes referred to as constant-amplitude variable phase-integrals. In this paper, we treat in detail only cases in which $F(x)$ is constant. In the introductory sections, we include a general $F(x)$ in order to indicate its role in a more sophisticated theory.

The approach we develop is straightforward in concept. It involves two stages. First we make a simple transformation to reduce the integral I_0 in (1.1) to one of form (1.2). Then we expand (1.2) in an asymptotic expansion in inverse powers of k.

In detail, however, things are far from straightforward. In the first stage, in order to effect the transformation, $G(x)$ must be monotonic in the integration interval (a, b). In practice, the original integral may have to be subdivided into sections in each of which $G(x)$ is monotonic and each section treated separately. When this subdivision has been carried out, we find that we are dealing with intervals (a, b) in which $G'(x)$ may be zero at one or both ends. It is the inverse of this function that is required to effect the transformation, and this may take several significantly different forms depending on whether or not $G'(a)$ or $G'(b)$ vanish. Sections 3 and 4 are devoted to information about inverse functions. We find that, depending on the vanishing of these derivatives, the function Φ in (1.2) may or may not have an algebraic singularity at an end point. If such a singularity is present, the standard asymptotic expansion (FCAE) is not valid. However, a different asymptotic expansion (see Theorem 5.1), due originally to Erdelyi, can be used. This is of a different form, and is given in detail in Section 5.

In Section 6 we apply the results of the two previous sections to construct an asymptotic expansion for I_0 in what we term the *flat symmetric ends* case. This is one in which $G'(a) = G'(b) = 0$ and $G''(a)G''(b) \neq 0$ and $G(x)$ is symmetric about both $x = a$ and $x = b$. Finally, in Subsection 7.1 we give a numerical example.

2 Background

2.1 Application

A practical application, which motivated this investigation, arises in the theory of three-dimensional pulse shaping for a photoinjector drive laser (Li and Lewellen [5]). The scheme uses laser phase and amplitude tailoring in combination with chromatic aberration of a dispersive lens to form a quasi-uniform ellipsoidal intensity distribution in the focal plane. Using a method based on Fourier optics, the intensity distribution for a spherical lens can be calculated by integrating the function

$$\exp\left[ik(R_1 - R_2 - \sqrt{R_1^2 - r^2} - \sqrt{R_2^2 - r^2})\right] \\ \times \left\{\exp[ik(\sqrt{r^2 + \nu^2 + z^2 - 2r\nu\cos\phi} - z)]\right\} \tag{2.1}$$

over a disc of radius R. A natural approach is to express this as a double integral

$$I(k) = \int_0^R \exp[ikH(r)] \left\{\int_0^\pi \exp[ik\, G(r, \phi)]d\phi\right\} rdr \tag{2.2}$$

and to use nested numerical quadrature.

The incidental parameters are

$$R_1 = R_2 = 150mm;\ R = 25mm;\ \nu = 2mm;\ z = 150mm.$$

The numerical values of the integral are required for values of k in the range $[0, 22520](mm)^{-1}$ Both functions $H(r)$ and $G(r, \phi)$, though of somewhat forbidding expression, have an innocent and harmless appearance when these incidental parameters are inserted.

For each value of k, one has to integrate a function over variable r in which each function value involves an integration over ϕ. For both integrations, standard one-dimensional quadrature routines are available. Numerical values for a range of values of k, both large and small, are required. For small values of k, this approach worked well. But for larger values, the cost became prohibitive. A calculation taking less than one second for small k was reported as taking 32 hours for k at the upper end of the range, and giving a suspect numerical result. This seems to be a consequence of using a polynomial-based, or a locally polynomial-based, integration routine for a highly oscillatory integrand.

Each function value for the outer integral requires a separate numerical evaluation of the inner integral. In this note, we are concerned only with the numerical evaluation of this *inner* integral. In Section 6, we derive an asymptotic expansion, using which this inner integral can be evaluated just as rapidly for large k as for small k. The coefficients in this expansion may have to be determined by using series inversion, which is treated in detail in Sections 3 and 4. To our knowledge, this problem (as stated in (2.1)) has not been completed. Only the inner integral described above is treated in this paper.

2.2 Recent literature

The numerical quadrature of highly oscillatory integrand functions has long been recognised as a major challenge. Until very recently, attention has been restricted to constant phase oscillators, those having constant $G'(x)$.

In the late nineteenth century, a common approach involved expanding the integral in what would nowadays be termed a truncated asymptotic expansion with a remainder term. Possibly the doyen of these is the FCAE which has a linear oscillator $G(x)$. In fact, Poisson used the FCAE (Theorem 5.2) in his proof of the Euler-Maclaurin expansion. These methods are valid for large k and require numerical values of $F(x)$ and its derivatives at the interval end-points.

In 1928, in a celebrated paper, Filon [2] developed a variant of Simpson's rule using weight function $\exp[ikG(x)]$ for these integrals. Naturally, this requires having available the values of the first few moments

$$\mu_m(k) = \int_a^b x^m \exp[ikG(x)]dx, \tag{2.3}$$

preferably in explicit form.

Recent developments, near the very end of the twentieth century led to the recognition that the appropriate numerical approach depends critically on the location of the points for which $G'(x) = 0$. These are termed critical points. In the earlier work $G'(x)$ is constant and there are no critical points.

More recently, amongst other results, Iserles has derived a generalisation of the FCAE for those oscillator functions $G(x)$ having no critical points in the integration interval. The coefficients depend on the early derivatives of $F(x)$ and $G(x)$ at the end-points and a very convenient recurrence for providing expressions for these coefficients is provided. The FCAE and this generalisation are classical in nature; they include inverse powers of k and may be established using integration by parts.

The asymptotic expansions mentioned above are valid only when $G(x)$ has no critical points, (points for which $G'(x) = 0$). When $G'(x)$ has critical points, the method of stationary phase can be exploited to provide corresponding expansions (which typically involve other inverse fractional powers of k). Explicit expressions for the coefficients in these expansions can be obtained using standard series inversion techniques. (See for example Section 4 below.) These are straightforward in concept, but are not well known. They can be tedious to apply. And, of course, specific forms of these coefficients are needed for direct numerical use.

In 2004, Iserles and Nørsett [4] published a powerful approach for these problems too. Using a technique akin to subtracting out the singularity, which could be described as suppressing the critical point contribution, the integral is expressed as the sum of two terms. One is an asymptotic expansion in inverse powers of k, not unlike one valid when there are no critical points. The other is a moment, $\mu_0(k)$, or, depending on the nature of the critical point, a weighted sum of several early moments.

The effect of these recent contributions is major. In cases where there are no critical points, or in which the moments are available, these problems may now be tackled successfully. But there remain problems, such as the one highlighted in this paper, in which there are critical points, and the integral $\mu_0(k)$ is not available. In fact, the problem treated in this paper is simply that of calculating $\mu_0(k)$ for large k.

2.3 Scaling

The integrals treated in this paper are all of the form

$$I_0 = \int_a^b F(x) \exp[ikG(x)]dx, \tag{2.4}$$

where

$$F(x), G(x) \in C^\infty[a, b]; \qquad G'(x) \neq 0 \quad \forall \quad x \in (a, b). \tag{2.5}$$

As a preliminary, we rescale the problem using elementary linear transformations. We find immediately

$$I_0 = (b - a) \exp[ikG(a)] \int_0^1 f(x) \exp[iKg(x)]dx, \tag{2.6}$$

where

$$f(x) = F(a + x(b - a)); \quad g(x) = (G(a + x(b - a)) - G(a))/(G(b) - G(a))$$

and

$$K = k(G(b) - G(a)).$$

The required properties (2.5) for $F(x)$, $G(x)$ over $[a, b]$ transform into identical properties for $f(x)$, $g(x)$ over $[0, 1]$. Thus, the initial problem (2.4) has been scaled to that of evaluating (2.6) where

$$f(x), g(x) \in C^{\infty}[0, 1]; \quad g'(x) > 0 \quad \forall \quad x \in (0, 1); \quad g(0) = 0; \quad g(1) = 1. \tag{2.7}$$

These conditions on $g(x)$ allow an elementary transformation $x = h(t)$, where

$$t = g(x) \tag{2.8}$$

in the integral which may be re-expressed in the form

$$I_2 = \int_0^1 f(h(t))h'(t) \exp[iKt]dt. \tag{2.9}$$

Here $h'(t)$ is the derivative of $h(t)$, the inverse function of $t = g(x)$. That is, $h(g(x)) = g(h(t)) = 1$ for all values of x and of t for which these expressions are defined.

The requirement that $g(x)$ be monotonic is needed so that this inverse function $x = h(t)$ is single valued and can be used to transform the integral.

At this point, we specialize to the case $F(x) = f(x) = 1$. In straightforward cases in which $g'(t)$ has no zeros, only marginal additional computation would be required to take into account the function $f(h(t))$. But, in general, $h(t)$ may have derivative singularities, so that, even when $f(x)$ is straightforward, complications introduced by these singularities into $f(h(t))$ may lead to a considerably more sophisticated theory. In this paper, we confine ourselves to the simpler theory, having $F(x) = 1$, that is, the *fixed-amplitude* variable phase integral.

3 Inverse functions

Interest then centers on the nature of the function $h'(t)$ where h is the inverse function of g. This appears to be critically dependent on the behavior of g at the end-points. For example, when $t = g(x) = g_1 x$, we find immediately that $x = h(t) = t/g_1$ In this case $h'(t)$ is a finite constant, and the FCAE (5.5) is available, leading to an asymptotic expansion in inverse powers of K. On the other hand, when $t = g(x) = g_2 x^2$, we find $x = h(t) = \sqrt{(t/g_2)}$. In this case $h'(t)$ has a weak singularity at $t = 0$. This implies we shall require at some point expansion (5.3) with $\alpha = -1/2$ leading to an expansion including half-integer inverse powers of K.

These remarks illustrate how the nature of the smooth function $g(x)$ at the end points plays a major role in the theory. The nature of the inverse function $h(t)$ determines the form of the asymptotic expansion through its derivative $h'(t)$.

In this paper we are addressing a situation in which $G(x)$ and by extension $g(x)$ are available in functional form. To exploit the asymptotic expansions in Section 5 we require information about $h'(t)$. A plot of $h(t)$ may be obtained by reflecting a plot of $g(x)$ about the line $t = x$.

In some cases one can proceed analytically to derive an analytic expression for $h(t)$. In Section 7 we report a numerical example with $(a, b) = (0, \pi)$ and

$$t = g(x) = (1 - \cos x)/2. \tag{3.1}$$

Elementary analysis leads to

$$x = h(t) = 2 \arcsin \sqrt{t} = \sqrt{t}(c_0 + c_1 t + c_2 t^2 + ...)$$

with

$$c_q = \frac{1.3...2q - 1}{2.4....2q} \frac{2}{2q + 1} \tag{3.2}$$

and

$$h'(t) = [t(1 - t)]^{-1/2} = t^{-1/2}\psi(t) = t^{-1/2}(\bar{c}_0 + \bar{c}_1 t + \bar{c}_2 t^2 + ...) \tag{3.3}$$

with

$$\bar{c}_q = (2q + 1)c_q/2.$$

In a similar manner one readily obtains

$$h'(t) = (1 - t)^{-1/2}\phi(t) = (1 - t)^{-1/2}(\bar{d}_0 + \bar{d}_1(t - 1) + \bar{d}_2(t - 1)^2 + ...). \tag{3.4}$$

In this particular example, $\bar{d}_q = (-1)^q \bar{c}_q$; these coefficients are needed in the asymptotic expansion in Section 5. The functions ψ and ϕ are termed the *regular* parts of h' at 0 and at 1 respectively.

4 Series inversion

Obtaining a simple analytic form for $h(t)$ is not to be expected. In point of fact, we need information about $h'(t)$ only at the end-points, and this can be obtained from information about $g(x)$ at the end points using series inversion. To do this we need only some of the early derivatives $g^{(s)}(0)$; these may be obtained readily from the analytic form of $g(x)$. Depending on the properties of $g(x)$, several different forms of series inversion may occur. In this section we describe some of them.

4.1 $g'(0) \neq 0$

When the power series

$$t = g(x) = g_1 x + g_2 x^2 + \dots \qquad g_1 \neq 0 \tag{4.1}$$

is absolutely convergent in a neighborhood of the origin, the inverse series

$$x = h(t) = b_1 t + b_2 t^2 + \dots \tag{4.2}$$

exists, is unique, and is also absolutely convergent in a neighborhood of the origin. Expressions for b_i in terms of g_i may be obtained by substituting (4.2) into (4.1) and comparing coefficients of powers of x. This gives;

$$\begin{aligned} b_1 &= 1/g_1, \\ b_2 &= -g_2/g_1^3 \\ b_3 &= (2g_2^2 - g_1 g_3)/g_1^5 \\ b_4 &= (-5g_2^3 + 5g_1 g_2 g_3 - g_1^2 g_4)/g_1^7 \end{aligned} \tag{4.3}$$

Naturally, the relations in (4.3) may be reversed by interchanging g_i and b_i throughout.

4.2 $g^{(s)}(0) = 0$ for all s odd; and $g''(0) \neq 0$

The previous development of $h'(t)$ is valid only when $g'(0) \neq 0$. When $g'(0) = 0$, these formulas no longer apply. We shall be interested in a particular special case in which in addition $g(x)$ is symmetric about $x = 0$, that is:

$$g'(0) = 0 \qquad g''(0) > 0 \qquad g^{(s)}(0) = 0 \qquad \forall\, s \text{ odd},$$

giving

$$t = g(x) = g_2 x^2 + g_4 x^4 + \ldots \qquad g_2 > 0. \tag{4.4}$$

This inversion can be related to the previous results simply by setting $X = x^2$, replacing (4.1) by

$$t = g_2 X + g_4 X^2 + \ldots \qquad g_2 \neq 0.$$

The result corresponding to (4.2) takes the form

$$X = b_1 t + b_2 t^2 + \ldots \qquad b_1 \neq 0.$$

Extraction of x provides two (equal and opposite) solutions. Restricting attention to positive t, we set

$$x = X^{\frac{1}{2}} = t^{\frac{1}{2}} (b_1 + b_2 t + \ldots)^{\frac{1}{2}},$$

which may be re-expressed in the form

$$x = h(t) = t^{\frac{1}{2}} (c_0 + c_1 t + c_2 t^2 + \ldots). \tag{4.5}$$

It appears the early coefficients are;

$$\begin{aligned} c_0 &= 1/g_2^{1/2}, \\ c_1 &= -g_4/2g_2^{5/2} \\ c_2 &= (7g_4^2 - 4g_2 g_6)/8g_2^{9/2} \\ c_3 &= (-33g_4^3 + 36g_2 g_4 g_6 - 8g_2^2 g_8)/16g_2^{13/2} \end{aligned} \tag{4.6}$$

These coefficients are used in the application in Section 6.

4.3 $g'(0) = 0$ and $g''(0) > 0$

The previous inversion depends on the symmetry of $g(x)$ about the origin. It is instructive to see how critical the nature of $g(x)$ at the end-point is to the solution. If, for example, $g'(0) = 0$ but the symmetry condition is not valid, we have to replace (4.4) by

$$t = g(x) = g_2x^2 + g_3x^3 + \dots \qquad g_2 > 0. \tag{4.7}$$

Using the same sort of manipulation as before, we find successively

$$\begin{aligned} t^{\frac{1}{2}} &= x(g_2 + g_3x + g_4x^2 + \dots)^{\frac{1}{2}} \\ &= x(a_1 + a_2x + a_3x^2 + \dots) \\ &= a_1x + a_2x^2 + a_3x^3 + \dots \end{aligned}$$

Applying the inversion that produced (4.2), we find

$$\begin{aligned} x = h(t) &= b_1t^{\frac{1}{2}} + b_2t + b_3t^{\frac{3}{2}} + \dots \\ &= t^{\frac{1}{2}}(b_1 + b_3t + b_5t^2 + \dots) \\ &\quad +(b_2t + b_4t^2 + b_6t^3 + \dots). \end{aligned} \tag{4.8}$$

4.4 $g^{(q)}(0) = 0$ for $q < r$; and $g^{(r)}(0) \neq 0$

One might not be surprised to encounter any of the three cases above. But it could happen that $G(x)$ has a horizontal point of inflexion, a situation in which $g'(0) = g''(0) = 0$. A more general result, based on

$$t = g(x) = \sum_{q \geq r} g_qx^q, \qquad g_r \neq 0, \tag{4.9}$$

is

$$x = h(t) = \sum_{j=1}^{\infty} b_jt^{j/r} = \sum_{j=1}^{r} t^{j/r}b^{[j]}(t), \tag{4.10}$$

each function $b^{[j]}(t)$ being regular at the origin.

5 Asymptotic expansions for fourier integrals

The key item in the theory of this paper is the asymptotic expansion in k for the Fourier coefficient $\hat{f}(k)$ of a function $f(x)$ that has algebraic singularities at the end points a and b but is otherwise regular. Let

$$f(x) = (x-a)^{\alpha}(b-x)^{\beta}r(x) \qquad \alpha, \beta > -1, \tag{5.1}$$

where $r(x)$ is analytic in a region containing $[a, b]$. We define the regular parts of $f(x)$ at the ends a and b respectively as

$$\psi(x) = (x-a)^{-\alpha}f(x), \quad \phi(x) = (b-x)^{-\beta}f(x). \tag{5.2}$$

Theorem 5.1 *When $f(x)$ is given by (5.1) and $\psi(x)$ and $\phi(x)$ are defined by (5.2), and $r(x)$ is analytic in a region containing the interval $[a,b]$, then for all positive integer p_1 and p_2*

$$\begin{aligned}\int_a^b f(x)e^{ikx}dx = & - e^{ikb-i\pi\beta/2}\sum_{q=0}^{p_1-1}\frac{\phi^{(q)}(b)i^{q+1}(q+\beta)!}{k^{q+\beta+1}\,q!} \\ & + e^{ika+i\pi\alpha/2}\sum_{q=0}^{p_2-1}\frac{\psi^{(q)}(a)i^{q+1}(q+\alpha)!}{k^{q+\alpha+1}\,q!} \\ & + O(k^{-(p_1+\beta+1)}) + O(k^{-(p_2+\beta+1)}) \quad as \quad k\to\infty. \end{aligned} \tag{5.3}$$

This result, which appeared in 1955, is attributed to Erdelyi [1] who established it using neutraliser functions and general integration by parts. Three years later, it was re-established by Lighthill [6], using generalised function theory. Erdelyi's proof requires only that $r(x)$ is $C^{p_j}(a,b)$ and need not be analytic. In 1971, a straightforward proof based on contour integration was published by Lyness [7].

A more familiar case of this theorem arises when one sets $\alpha = \beta = 0$, making $f(x)$ analytic in $[a,b]$. This reduces to a classical expansion, which may be established independently using integration by parts. Iterating the relation

$$\int_a^b f(x)\exp[ikx]dx = \frac{e^{ikb}f(b) - e^{ika}f(a)}{ik} - \frac{1}{ik}\int_a^b f'(x)\exp[ikx]dx \tag{5.4}$$

we readily establish the following classical theorem.

Theorem 5.2 (FCAE) *For all positive integer p, and $k > 0$, when $f(x) \in C^{(p)}(a,b)$*

$$\begin{aligned}\int_a^b f(x)e^{ikx}dx = & - e^{ikb}\left\{\frac{i}{k}f(b) + \frac{i^2}{k^2}f'(b) + \cdots + \frac{i^p}{k^p}f^{(p-1)}(b)\right\} \\ & + e^{ika}\left\{\frac{i}{k}f(a) + \frac{i^2}{k^2}f'(a) + \cdots + \frac{i^p}{k^p}f^{(p-1)}(a)\right\} \\ & + \frac{i^p}{k^p}\int_a^b f^{(p)}(x)e^{ikx}dx. \end{aligned} \tag{5.5}$$

The previous theorem reduces to this one when both α and β are nonnegative integers. In fact, the remainder term in (5.3) can be expressed as a sum of contour integrals that, of course, reduces to the straightforward remainder term in (5.5) in the simpler case.

6 The flat symmetric ends case

All integrands treated in this paper satisfy (2.7) namely,

$$g(x) \in C^{\infty}[0,1]; \quad g'(x) > 0 \quad \forall \quad x \in (0,1); \quad g(0) = 0; \quad g(1) = 1. \tag{6.1}$$

Possibly the most common special case (which occurs naturally in the inner integral case (2.1)) is one in which, in addition,

$$\begin{aligned} g'(0) = g'(1) = 0; &\qquad g''(0).g''(1) < 0; \\ g(-x) = g(x); &\qquad g(1-x) = g(1+x). \end{aligned} \tag{6.2}$$

These conditions assert that $g(x)$ is flat at both ends and is symmetric about each end.

To proceed, we need numerically based information about the derivative of $h(t)$, the inverse function of $g(x)$. This function $g(x)$ satisfies precisely the conditions specified in Subsection 4.2 both at the end $x=0$ and at the end $x=1$. Reference to (4.5) shows that $h(t) \in C^{\infty}(0,1)$ but that $t^{-1/2}h(t)$ is regular at $t=0$. A corresponding examination of the form of $h(t)$ at $t=1$ gives the same situation; that is, $(1-t)^{1/2}h(t)$ is regular at $t=1$. It follows that $h(t)$ has the form $h(t) = t^{1/2}(1-t)^{1/2}\bar{h}(t)$, where $\bar{h}(t) \in C^{\infty}[0,1]$. (Incidentally, as indicated in Section 4, $h(t)$ is *not* of this form unless *both* symmetry conditions in (6.2) are satisfied.) From this, it follows that

$$h'(t) = t^{-1/2}(1-t)^{-1/2}r(t), \tag{6.3}$$

where $r(t)$ is $C^{\infty}[0,1]$.

With $f(x) = 1$, the integral in (2.9) reduces to

$$\begin{aligned} I_2 &= \int_0^1 \exp[iKg(x)]\,dx = \int_0^1 h'(t)\exp[iKt]\,dt \\ &= \int_0^1 t^{-1/2}(1-t)^{-1/2}r(t)\exp[iKt]dt. \end{aligned} \tag{6.4}$$

The reader will recognize this final integral as a special case of the one expanded in Theorem 5.1, obtained by applying it to $f = h'$ in (6.3) with parameters $a=0, b=1, \alpha=\beta=-1/2$. Replacing this integral by its asymptotic expansion (5.3) we obtain the principal result in this paper:

$$\int_0^1 \exp[iKg(x)]dx = \sum_{q=0}^{s} \frac{-e^{iK}T_q(1) + T_q(0)}{K^{q+\frac{1}{2}}} + O(K^{-s-\frac{3}{2}}), \tag{6.5}$$

where

$$T_q(1) = e^{i\pi/4}\,\frac{\phi^{(q)}(1)}{q!}\,i^{q+1}\left(q-\frac{1}{2}\right)! \qquad T_q(0) = e^{-i\pi/4}\,\frac{\psi^{(q)}(0)}{q!}\,i^{q+1}\left(q-\frac{1}{2}\right)!. \tag{6.6}$$

and ϕ and ψ are the regular parts of $h'(t)$ at the end points, namely

$$\psi(t) = t^{1/2}h'(t), \quad \phi(t) = (1-t)^{1/2}h'(t). \tag{6.7}$$

These coefficients are obtained from $G(x)$ as follows: Inverting the series $t = g(x)$ as explained in Subsection 4.2 will provide the numerical values of the coefficients in

$$x=h(t)=t^{\frac{1}{2}}(c_0+c_1t+c_2t^2+\ldots)=(1-t)^{\frac{1}{2}}(d_0+d_1(t-1)+d_2(t-1)^2+\ldots). \quad (6.8)$$

In the asymptotic expansion (6.5) we need the Taylor Coefficients $\bar{c}_q$ of $\psi(t) = t^{\frac{1}{2}}h'(t)$ and $\bar{d}_q$ of $\phi(t) = (1-t)^{\frac{1}{2}}h'(t)$ and these are

$$\frac{\psi^{(q)}(0)}{q!} = \bar{c}_q = \left(q+\frac{1}{2}\right)c_q, \qquad \frac{\phi^{(q)}(1)}{q!} = -\bar{d}_q = -\left(q+\frac{1}{2}\right)d_q$$

respectively. Substituting this into (6.5) yields.

Theorem 6.1 *When the oscillator function $G(x)$ satisfies the conditions :*

$$G(x) \in C^{\infty}[a,b]; \quad G'(x) > 0 \quad \forall \quad x \in (a,b); \quad G'(a) = G'(b) = 0;$$

$$G''(a).G''(b) < 0; \quad G(a-x) = G(a+x); \quad G(b-x) = G(b+x). \quad (6.9)$$

then

$$\int_a^b \exp[ikG(x)]dx = -\,e^{ikG(b)+i\pi/4}\sum_{q=0}^{s}\frac{i^{q+1}(q+\frac{1}{2})!}{K^{q+\frac{1}{2}}}D_q$$
$$+\,e^{ikG(a)-i\pi/4}\sum_{q=0}^{s}\frac{i^{q+1}(q+\frac{1}{2})!}{K^{q+\frac{1}{2}}}C_q + O(K^{-s-\frac{3}{2}}), \quad (6.10)$$

where $K = k(G(b) - G(a))$ and $C_q = (b-a)c_q$ and $D_q = (b-a)d_q$ where c_q and d_q are defined in (6.8) *above.*

Equations (6.5) and (6.10) are identical in content. The second form is set in a coordinate system in which the problem is likely to be encountered. That is C_q is a Taylor coefficient related to the inverse of $G(x)$. It may be obtained directly from G_j the Taylor coefficient of $G(x)$ at $x = a$ using (4.6) the same formulas as those relating c_q with g_j.

Note that these are *asymptotic* expansions. Trivial cases apart, they do not converge. For large K the terms first diminish and then increase. Also there is no reason to suppose that they are semi-convergent. That is, in general the truncation error is *not* necessarily bounded by the first omitted term.

7 Notes on application

For all k or K, the integrals I_0 or I_1 may be approximated by applying an n-panel trapezoidal rule (Table 1)

$$R^{[n]}[a,b]f = \frac{b-a}{n}\sum_{j=0}^{n}{}'' f\left(a+\frac{(b-a)j}{n}\right) \quad (7.1)$$

either in (2.4) directly or in (2.6). One way of organizing this is to calculate $R^{[1]}f$, $R^{[2]}f$, $R^{[4]}f$, accepting the result when $|R^{[k]}f - R^{[k/2]}f| < \epsilon$, the required tolerance. Other rules and strategies can be used. But for larger k or K, this approach and others of the same character may become too expensive. In general, the trapezoidal rule is needed for small k and is of occasional use for large k as a check on the overall result to verify the programming of the asymptotic expansion coefficients.

To apply the theory in this paper, the user must first subdivide his integral (2.4) at all points where $G'(x) = 0$. The method is viable only to the extent that this a step is carried out exactly. We note that the contributions to the asymptotic expansion arise only from the interval end-points and from points where $G'(x) = 0$. The behavior of $G(x)$ in between these points affects the result only through the derivatives of G at these points which occur in the coefficients. Moreover, further subdivision at a point where $G'(x) \neq 0$ affords no advantage, since the contribution from this point to the interval on the left is equal and opposite to the corresponding contribution to the interval on the right.

In the examples, we treat a flat symmetric ends case using the asymptotic expansion of the previous section. This particular oscillation function has been discussed in Section 3 where the expansion coefficients $\psi^{(q)}(0)/q! = \bar{c}_q$ and $\phi^{(q)}(1)/q! = \bar{d}_q$ may be obtained analytically from the oscillator $g(x)$.

7.1 Remarks on the numerical example

In the example, we have restricted ourselves to values of K for which all results are real. In general all entries in these tables would be complex numbers.

We note the behavior of the "brute force" trapezoidal rule approximations. The results appear to be arbitrary until n exceeds K/π when they rapidly converge. (This convergence is not really as sudden as it seems. We are doubling the value of n at each entry.)

Tables 2, 3 and 4 outline some of the steps taken in using the asymptotic expansion. The calculation of the four coefficients in Table 2 may be a significant undertaking. Once this is done, evaluation of the truncated asymptotic series (illustrated in Tables 3 and 4) requires little more than the evaluation of a cubic in K^{-1}. The final lines in Table 1 and in Table 4 are approximations to the integral. Undoubtedly, the final entries in Table 1 give the correct results to the number of figures shown. Comparison of these with the entries in Table 4 illustrates the quality of the truncated asymptotic expansion. For small K, the trapezoidal rule provides economic approximations, (8 or 16 function values) while the corresponding results in Table 4 are not convincingly accurate. For larger values of K, the trapezoidal rule approximations are expensive (perhaps $2K$ function values), while the truncated asymptotic series if anything, becomes cheaper. In making these comparisons, one should bear in mind that, for each value of K a separate trapezoidal rule evaluation is necessary, requiring n function values. However, once the values of $T_q(0)$ and $T_q(1)$ are available, evaluation for any large value of K uses the same coefficients and requires a single calculation of a cubic. In problems such as the one described in Section 2, this may represent a simply enormous gain in efficiency.

7.2 Numerical examples

We report approximations to four integrals, namely

$$\int_0^{\pi} \exp[iK(1-\cos x)/2]dx$$

with $K = 2\pi, 8\pi, 128\pi$ and 800π.

Table 1 Approximations using n-panel trapezoidal rule (7.1)

n	$K=2\pi$	$K=8\pi$	$K=128\pi$	$K=800\pi$
8	0.95580499	0.639724837	−0.46355326	−0.543395827
16	0.95580499	0.494824067	−0.746887558	0.524104174
32	0.95580499	0.494824067	−0.196868068	0.132966687
64	0.95580499	0.494824067	−0.183399531	−0.105532816
128	0.95580499	0.494824067	0.124922071	0.194571162
256	0.95580499	0.494824067	0.124922071	0.200483897
512	0.95580499	0.494824067	0.124922071	0.230534403
1024	0.95580499	0.494824067	0.124922071	0.0499950242
2048	0.95580499	0.494824067	0.124922071	0.0499950242

Table 2 The asymptotic series coefficients: values of $(-e^{iK}T_q(1)+T_q(0))$

q	all even K/π
0	2.50662827
1	−0.626657069
2	−0.704989202
3	1.4687275

Table 3 The asymptotic series: individual terms, values of $(-e^{iK}T_q(1)+T_q(0))/K^{q+1/2}$

q	$K=2\pi$	$K=8\pi$	$K=128\pi$	$K=800\pi$
0	1.	0.5	0.125	0.05
1	−0.03978873580	−0.00497359197	−7.77123746E-05	−4.97359197E-06
2	−0.00712414572	−0.00022262955	−2.17411674E-07	2.22629554E-09
3	0.00236217293	1.8454476E-05	1.12637183E-09	1.8454476E-12

Table 4 Truncated asymptotic series evaluation: values of $\sum_{q=0}^{s}(-e^{iK}T_q(1)+T_q(0))/K^{q+1/2}$

s	$K=2\pi$	$K=8\pi$	$K=128\pi$	$K=800\pi$
0	1.	0.5	0.125	0.05
1	0.960211264	0.495026408	0.124922288	0.0499950264
2	0.953087119	0.494803778	0.124922071	0.0499950242
3	0.955449291	0.494822233	0.124922071	0.0499950242

8 Concluding remarks

This paper extends slightly the availability of asymptotic expansions for the evaluation of integrals

$$I_0 = \int_a^b F(x) \exp[ikG(x)]dx, \tag{8.1}$$

for large k. We consider only cases in which $F(x), G(x) \in C^{(\infty)}[a, b]$ and $G'(x) \geq 0$ in $[a, b]$; in which the moment integrals are not available; the coefficients in these asymptotic expansions have straightforward expressions in terms of low order derivatives of F and of G at a and at b. In 2004, Iserles and Nørsett [4] have provided an asymptotic expansion in inverse powers of k, valid only for G satisfying $G'(a)G'(b) > 0$. In this paper, a corresponding expansion, in inverse half integer powers of k is derived for the cases in which $F(x) = 1$, $G'(a) = G'(b) = 0$, but $G''(a)G''(b) < 0$, and $G(x)$ is symmetric both about a and about b.

The approach described here is direct, making no explicit appeal to the theories of stationary phase or steepest descent. This approach may be readily generalised to a wide range of problems, in some of which both $F(x)$ and $G(x)$ may have algebraic singularities at the end points. The case treated here is perhaps the simplest non-trivial case.

Finally, I would like to thank Dr. Iserles for, at an earlier stage, encouraging me to consider this sort of problem and to thank Dr Huybrechs for significant encouragement, for keeping me abreast of the recent literature (see e.g. [3]) and for making sure that a proper application of the Stationary phase approach does indeed reveal the same result.

Acknowledgements The author was supported by the Mathematical, Information, and Computational Sciences Division subprogram of the Office of Advanced Scientific Computing Research, Office of Science, U.S. Department of Energy, under Contract DE-AC02-06CH11357.

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